# Approaches to modelling local nitrogen deposition and concentrations in the context of Natura 2000 - Topic 4

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# 1. Introduction

Atmospheric nitrogen loading of nature areas is both a local and a transboundary problem. Contributions from mainly wet deposition of long-range transported aerosol bound nitrogen compounds in some regions already exceed the critical loadings of sensitive ecosystems. Close to intensive agricultural areas the contribution from dry deposition of locally emitted ammonia may, however, equal or even exceed the nitrogen contribution from long-range transport. The assessment of atmospheric nitrogen deposition needs therefore to account for both local and long-range transport contributions to the atmospheric nitrogen input to the nature area in question[1].

Table 1 State-of-the-art in modelling long-range-transport and local scale nitrogen deposition[1].

| Area | Long-range transport | Local scale |
|---|---|---|
| **Emissions** | European 17 km x 17 km inventory. For parts of the domain including detailed seasonal variation. | Inventory on single farm level with dynamic seasonal variation and separated on contribution from stables, manure application |
| **Transport** | Eulerian 2-way nested grid models with 17 km x 17 km or even 5 km x 5 km resolution in the inner nest. | Gaussian or Lagrangian dispersion with a spatial resolution of e.g. 1-500 m. For modelling flows around building etc, CFD models can be used. However, these models tend to need site specific calibration so are not amenable to routine use. |
| **Aerosol description** | Dynamic aerosol phase chemistry. | First-order transformation between gas phase $NH_3$ and aerosol phase $NH_4^+$. |
| **Gas phase chemistry** | Explicit chemical mechanisms including the most important species. | First-order transformations. |
| **Wet deposition** | Full wet phase chemistry in cloud and rain droplets and subsequent scavenging of rain droplets. | Simple wash out ratios for both gases and particles |
| **Dry deposition** | Resistance method with detailed seasonal variations in surface resistance and accounting for current meteorological conditions. Bi-directional flux parameterisation for $NH_3$. | Resistance method with detailed seasonal variation in surface resistances and accounting for current meteorological conditions and spatial variation of land use. Bi-directional flux parameterisation for $NH_3$. |

It should be noted that Natura 2000 areas vary considerably in size throughout Europe – from few hundreds of meters in depth to many kilometres. This has, of course, implications on which tools are applicable. The focus in the current chapter is on describing the model approaches in assessment of local atmospheric nitrogen deposition. We limit ourselves to describing the contribution from local sources within a distance of 1 to 20 km.

## 1.1. Processes on the local scale

In the following we will look into which processes that play a major role and therefore need to be included on the local scale.

*Chemical transformation*

Only fast chemical transformations can take place on a time scale of minutes to a couple of hours (transport time within the modelling domain). This applies to the NO to $NO_2$ conversion in reaction with ozone and the photo dissociation of $NO_2$ reforming NO. The conversion from $NO_2$ to $HNO_3$ in reaction with hydroxyl (OH) radical has a rate of about 5% per hour, which means that this reaction is negligible on this time scale. $NH_3$ reacts with acid gases and aerosols in the atmosphere in the formation of aerosol phase ammonium ($NH_4^+$). In the 1980s and 1990s the average conversion rates in Europe have been estimated to be in the order of 30% per hour, but due to the large reductions in European sulphur emissions leading to significant decrease in sulphate concentrations, the conversion rate is now believed to be on the order of 5% per hour[2]. Thereby also $NH_3$ to $NH_4^+$ conversion may for most practical purposes be disregarded in local scale modelling.

*Dry deposition*

It is common to assume a zero concentration on the ground in the computation of the dry deposition flux. This, however, may not apply over vegetation where the flux of $NH_3$ and $NO_2$ may be bi-directional. This bi-directional flux depends on the concentration in the air as well as in the plants, which again changes during the season and due to management such as grass cutting or use of fertilizer. An important pathway for dry deposition of $NH_3$ is the uptake through stomata of plants, but it may also be absorbed through dew on the plants or through the thin water film on the leaves epidermis[3]. Experimental studies have shown that a co-deposition of $NH_3$ and $SO_2$ takes place, and that the ratio between atmospheric concentrations of these two compounds together with the humidity and temperature are important factors for the deposition of $NH_3$[4]. $NO_2$ may also be taken up by the plants through the stomata. Although this deposition is not very fast (to a forest the dry deposition velocity is of the order of 2 to 4 mm/s), it may in some areas be of importance for the overall atmospheric nitrogen deposition[5]. $HNO_3$ sticks to almost any surface and is therefore, quickly deposited. In addition, the dry deposition of peroxyacetyl nitrate (PAN), $N_2O_5$, and HONO may be of some importance for the overall nitrogen deposition[5]. As previously discussed, the formation of these $NO_y$ compounds is too slow for local emissions to play a role in the atmospheric deposition of nitrogen.

*Wet deposition*

Precipitation events take place only during a very limited part of the time. The residence of local pollutants within the 10 to 20 km distance from the source is on the order of minutes to a couple of hours. This means that within this domain wet deposition of locally emitted pollution is generally negligible and it may therefore for most purposes be disregarded in local scale modelling of nitrogen deposition[1].

*Transport*

Buildings and other obstacles can have significant influence on the initial dispersion of $NH_3$ downwind from livestock houses. The landscape may also impose certain flow conditions that have to be accounted for and the local vegetation may influence the generation of turbulence and thereby affect the rate of dispersion. Topography also affects local-dispersion and if the slope of the modelling domain is significant (e.g. > 10%) then it should be included in the simulation.

### 1.2. Current state-of-the-art in modelling

Above we have discussed the processes that need to be accounted for in modelling of the local scale nitrogen deposition. Table 1 summarises state of the art in process descriptions of currently applied models. For comparison modelling on long-range transport is also included in the table.

## 2. Methodologies and tools

In the following section we will outline the main features of model tools and systems applied in the literature. Concerning approaches in calculating nitrogen loadings of nature areas one may distinguish between methods and tools developed for:

- Screening models – to provide a crude and quick assessment of the potential environmental impact of nitrogen loadings
- Methods based on nomograms and tables generated from model calculations of source-receptor relationships
- Application of detailed model systems

Simple screening may be based on simple parameters like distance between sources and nature area and crude worst case deposition estimates. A recent example of a screening model is SCAIL, which was developed to provide screening estimates for ammonia concentration/deposition near to agricultural sources[x]. Nomograms and tables are even simpler and somewhat crude tools in estimating the loads, but in some countries these are officially accepted tools according to the local legislation and applied by local authorities and consultants; e.g. for Denmark. Our focus in this context is mainly on the detailed model systems. These detailed model systems are listed in Table 2.

Table 2 Models applied in local scale modelling of nitrogen deposition.

| Name | Type of model | Process description | Refs |
|---|---|---|---|
| **AERMOD** | Advanced plume model. | Uses hourly meteorological data from which atmospheric stability and dispersion parameters are derived. Handles ground and elevated sources in both simple and complex terrain. Dry deposition using the source depletion and applying the resistance algorithm. Wet deposition is implemented using simple wash out ratios for both gases and particles. Option for use seasonal variation of resistances | 6 |
| **ADMS** | Advanced plume model. | Uses hourly meteorological data from which atmospheric stability and dispersion parameters are derived. Handles ground and elevated sources in both simple and complex terrain. Dry deposition using a user-specified deposition velocity. Wet deposition is implemented using simple wash out ratios for both gases and particles Dry and wet deposition algorithm recently updated. | 7 |
| **FRAME** | Lagrangian transport model. | The FRAME (Fine Resolution Ammonia Exchange) model. Horizontal resolution grid of 5 km x 5 km and 33 vertical grid layers. Boundary conditions from FRAME-Europe on 150km x 150km resolution. The model is calibrated to deposition to interpolated mapped depositions on cell basis using measurements averaged over three recent years. Dry deposition applying the resistance method and five land use classes. Wet deposition applying scavenging ratios adopted from the EMEP (European Monitoring and Evaluation Programme) Eulerian long-range chemistry-transport model and implementing a directional orography rain fall model for enhanced precipitation resulting from terrain. | 8 |

| | | | |
|---|---|---|---|
| **CMAQ** | Eulerian chemistry-transport model | The model is constructed for use of meteorology provided by the MM5 meteorological model, but other sets of meteorological data may also be applied. Full Carbon-Bond V (CB05) chemical mechanism including an aerosol module derived from the Regional Particulate Model (RPM). The CMAQ is a multi-layer model with variable resolution and includes a sub-grid scale treatment at a finer spatial resolution than the grid being modelled of chemistry and dynamics of selected large point source plumes (PinG). Hourly dry deposition computed using the resistance methods adopted from the RADM scheme applying 11 land use types and including seasonal variations. Wet deposition in is modelled using scavenging coefficients. http://www.cmaq-model.org/ | 9 |
| **LADD** | Lagrangian multi-layer model | The LADD (Local Area Dispersion and Deposition) model builds upon the trajectory approach from the FRAME model. The horizontal resolution is 50m x 50m and with a very high vertical resolution (lowest grid points defined at 0.25m; 0.5m; 1.0m and 2.0m above ground. The model computes dry deposition of $NH_3$ applying the resistance method. Wet deposition is not accounted for in the model. | 10, 11 |
| **DEHM** | Eulerian chemistry-transport model | The model is constructed for use of meteorology provided by the MM5 meteorological model, but other sets of meteorological data may also be applied. The model contains an explicit chemistry mechanism with about 80 species and 200 reactions. The model domain covers the entire Northern Hemisphere with a 150km x 150km grid resolution, but applying nested grid algorithms with a 50km x 50km resolution for Europe, and a 5kmx5km resolution for Denmark and close surroundings. Hourly dry deposition is computed using the resistance method in a version adopted from the EMEP model. Wet deposition is modelled applying in-cloud and below-cloud scavenging coefficients. | 12-14 |
| **OPS** | Gaussian plume model on the local scale and Lagrangian transport further away from the source. | Makes use of statistical climatology derived from hourly meteorological mast data. Computations are performed for the different defined classes and hourly concentrations and depositions are derived from weighting according to the frequency. Chemistry is handled using first order conversion rates. The dry deposition is described based on a height independent deposition flux as a product of the vertical deposition speed at a specific height (50 meter) and the concentration at that height. The wet deposition is described as wash out and rain out: wash out is modelled with the aid of a washout coefficient, rain out happens after the plume has penetrated the cloud and thus at greater distances from the source. A short-term local-scale version of the model has also been developed (OPS-st). | 2, 15, 16, x |
| **OML-DEP** | Gaussian plume model. | Uses hourly meteorological data from which atmospheric stability and dispersion parameters are derived in a pre-processor. Handles point and area sources in simple terrain and applying variable horizontal resolution (usually 400m x 400m but also 100m x 100m has been applied). Dry deposition is parameterised by surface depletion and applying resistance algorithm. No wet deposition and no bi-directional flux parameterisations are implemented. | 1, 17, 18 |

# 3. Impact of local legislation

Local legislation is a powerful tool for reducing local atmospheric nitrogen loading of nature areas. These regulations may include use of buffer zone around sensitive nature areas, restrictions on number of animal units per farm etc. Trees have been discussed as a tool in landscape planning to reduce the impact of atmospheric $NH_3$ deposition, and local scale models have been used to evaluate the impact[19, x].

## 3.1. Denmark

Danish legislation includes demands for the so-called harmonisation areas; meaning that the livestock farm needs to include or have access to field areas of the necessary size for application of the produced manure in compliance with maximum nitrogen input on the field. The Danish animal production is intensive and in calculations of the nitrogen loadings of Danish nature areas, it is thus a good assumption that farmers apply the maximum manure on all grown fields. Another Danish restriction is that application has to take place when plants have the maximum nitrogen uptake. This is during growth and in practice this means that most application takes place during a short time period in spring. Danish model studies have demonstrated that the temporal variation in $NH_3$ emissions[20, 21] needs to be accounted for in order to reproduce the pattern in $NH_3$ concentrations and deposition.

Increasing the animal production in Danish farms has to be approved by the local municipality. The application is treated using a nomogram method for estimating local $NH_3$ deposition to nature areas in the nearby surroundings. These nomograms are used to estimate the deposition as function of distance from the source (farm housing, storage or fields with manure application). The nomograms are generated from model calculations[22] performed with the Danish OML-DEP Gaussian plume model.

# 4. Model validation studies

Local scale models have been tested against campaign measurements from a number of European field studies. Table 3 provides a list (*only one now but more will be added*) of such validation studies in literature.

Table 3 Model validation studies in literature concerning local atmospheric nitrogen deposition.

| Country | Model | Type of validation | Input & characteristics | Perform | Refs |
|---|---|---|---|---|---|
| **DK** | OML-DEP | Dry deposition of $NH_3$ from one poultry farm and one pig farm. Was deposition actually measured? If not then this is not a true validation. | Metdata from local mast established for experiment. | fair | [18] |
| **More to be added** | .. | .. | .. | .. | .. |

# 5. Experience from selected countries

Examples of assessment studies using local scale model tools are given below for a number of European countries. Table 4 lists some selected assessment studies from European countries. It is seen that most of these studies are from Denmark, The Netherlands, and UK?...

Table 4 Selected assessment studies concerning local scale atmospheric nitrogen deposition.

| Country | Model | Type of assessment | Input & characteristics | Refs |
|---|---|---|---|---|
| **UK** | UK-ADMS 3.1 | Dry & wet deposition of $NH_3$ from broiler chicken (225000) farm. | 10 yrs mast met data. EF: 2.8 g $NH_3$-N/hr/LU. No background. No terrain correction. | |
| **UK** | AERMOD PRIME | Deposition of $NH_3$ from broiler chicken (112,500 & 225,000) farm. | 1995 mast met data. Emis: 0.05 kg $NH_3$/broiler place/yr. No terrain correction. Background: www.apis.ac.uk. | |
| **UK** | UK-ADMS 3.3 | Deposition of $NH_3$ from broiler chicken (5,000) | 2002-2006 mast met data. Emis: 0.05 kg $NH_3$/broiler place/yr, 4.13 kg $NH_3$/tonne | |

| | | | | |
|---|---|---|---|---|
| | | farm. | spread & 2.38 kg $NH_3$/tonne storage. No terrain correction. Background incl. without ref. | |
| **UK** | ISC-AERMOD | Scenario studies of dry & wet deposition of $NO_x$ (+other) from animal rendering facility. | 12, 20 and 30 m stacks plus generator emissions. 2001-2005 mast met data. Building downwash. Investigation for calm conditions (ws 1 m/s). Rural surface. Background: www.apis.ac.uk. | |
| **UK** | AERMOD PRIME & ADMS | Scenario studies of worst case long-term dry deposition of $NO_x$ (and $SO_2$) from waste incinerator producing heat and power. | 80 m stack. ADMS fixed surface roughness (0.02 m) AERMOD: land use dep., Building downwash. $V_d$ $NO_2$ (0.0015m/s). Background: www.apis.ac.uk. | |
| **DK** | DAMOS (DEHM + OML-DEP) | Mapping of atmospheric nitrogen depositions to selected sensitive nature areas in two local administrative regions. | $NH_3$ emissions from fields, animal housing and storage facilities from all farms within 16 km x 16 km domain around the nature area. | [25, 26] |

**Denmark**

The atmospheric nitrogen load of Danish land and sea surfaces are mapped within the national monitoring programme for water and nature (NOVANA). The background atmospheric nitrogen deposition on 17 km x 17 km is computed using the Danish Eulerian Hemispheric Model (DEHM), and for selected nature areas detailed mappings of $NH_3$ depositions on 400 m x 400 m are performed using the OML-DEP model[23]. The resolution in the DEHM computations will soon be increased to 5 km x 5 km. The combination of DEHM and OML-DEP is called DAMOS – the Danish Ammonia Modelling System[1, 24].

*More countries to come*

## 6. Conclusions

Transport-chemistry models are strong tools in environmental assessment of atmospheric nitrogen loads…

## 7. Key Questions for Discussion

1. How comparable are modelling approaches of different European countries?
2. What are the current uncertainties in the modelled estimates of concentrations and deposition?
3. What model developments or data requirements are needed to reduce these uncertainties?
4. How can model uncertainties be taken into account?
5. How should model outputs be used/presented in impact assessments?

## 8. References

1. Hertel O, Skjøth CA, Løfstrøm P et al. Modelling Nitrogen Deposition on a Local Scale - A Review of the Current State of the Art. Environ Chem 2006; 3(5):317-337.

2. Van Jaarsveld H. The Operational Priority Substances model: Description and validation of OPS-Pro 4.1. 500045001. 2004. Bilthoven, The Netherlands, National Institute for Public Health & Environment. RIVM Report.
Ref Type: Report

3. Nemitz E, Sutton MA, Wyers GP, Jongejan PAC. Gas-particle interactions above a Dutch heathland: I. Surface exchange fluxes of NH3, SO2, HNO3 and HCl. Atmospheric Chemistry and Physics 2004; 4:989-1005.

4. Neirynck J, Kowalski AS, Carrara A, Ceulemans R. Driving forces for ammonia fluxes over mixed forest subjected to high deposition loads. Atmospheric Environment 2005; 39(28):5013-5024.

5. Wesely ML, Hicks BB. A review of the current status of knowledge on dry deposition. Atmospheric Environment 2000; 34(12-14):2261-2282.

6. US-EPA. AERMOD Deposition Algorithms - Science Document. -22. 2004.
Ref Type: Report

7. Carruthers DJ, Holroy DRJ, Hunt JCR et al. Uk-Adms - A New Approach to Modeling Dispersion in the Earths Atmospheric Boundary-Layer. Journal of Wind Engineering and Industrial Aerodynamics 1994; 52(1-3):139-153.

8. Griffith SJ. Analysis of modelled 2010 deposition results from FRAME and comparison with results from other models. Joint Environment Programme, PT/06/BE1772/R. 2007.
Ref Type: Report

9. Binkowski FS, Roselle SJ. Models-3 community multiscale air quality (CMAQ) model aerosol component - 1. Model description. Journal of Geophysical Research-Atmospheres 2003; 108(D6).

10. Dragosits U, Theobald MR, Place CJ et al. Ammonia emission, deposition and impact assessment at the field scale: a case study of sub-grid spatial variability. Environmental Pollution 2002; 117(1):147-158.

11. Sutton MA, Milford C, Dragosits U et al. Dispersion, deposition and impacts of atmospheric ammonia: quantifying local budgets and spatial variability. Environmental Pollution 1998; 102(1, Supplement 1):349-361.

12. Christensen JH. The Danish Eulerian hemispheric model - A three-dimensional air pollution model used for the Arctic. Atmospheric Environment 1997; 31(24):4169-4191.

13. Frohn LM, Christensen JH, Brandt J. Development and testing of numerical methods for two-way nested air pollution modelling. Physics and Chemistry of the Earth 2002; 27(35):1487-1494.

14. Frohn LM, Christensen JH, Brandt J. Development of a high-resolution nested air pollution model - The numerical approach. Journal of Computational Physics 2002; 179(1):68-94.

15. Pul Av, Jaarsveld HV, Meulen Tvd, Velders G. Ammonia concentrations in the Netherlands: spatially detailed measurements and model calculations. Atmospheric Environment 2004; 38(24):4045-4055.

16. Colles A, Janssen L, Mensink C. Optimalisation OPS model. Combined report for the OPS-maintenance contract part 3 and the MIRA O&O contract 2003. VITO-report 2004/IMS/R/038. 2004.
Ref Type: Report

17. Dop Hv&KG, editor. An Improved Dispersion Model for Regulatory Use - The OML Model.: Plenum Press; 1992.

18. Sommer SG, Østergård HS, Løfstrøm P, Andersen HV, Jensen LS. Validation of model calculation of ammonia deposition in the neighbourhood of a poultry farm using measured NH3 concentrations and N deposition. Atmospheric Environment 2009; 43(4):915-920.

19. Smithers R, editor. The role of trees in landscape planning to reduce the impacts of atmospheric ammonia deposition. 00 Oct 1; IALE(UK)/Woodland Trust, Grantham; 2004.

20. Gyldenkærne S, Skjøth CA, Hertel O, Ellermann T. A dynamical ammonia emission parameterization for use in air pollution models. Journal of Geophysical Research-Atmospheres 2005; 110(D7).

21. Skjøth CA, Hertel O, Gyldenkærne S, Ellermann T. Implementing a dynamical ammonia emission parameterization in the large-scale air pollution model ACDEP. Journal of Geophysical Research-Atmospheres 2004; 109(D6).

22. Geels C, Bak J, Callesen T et al. Guideline for approval of livestock farms (In Danish: Vejledning om godkendelse af husdyrbrug). 568, -83 p. 2006. Roskilde, Denmark, National Environmental Research Institute.
Ref Type: Report

23. Ellermann T, Andersen HV, Bossi R et al. Atmospheric Deposition 2006. NOVANA (In Danish: Atmosfærisk Deposition. NOVANA). No. 645, -65p. 2007. Roskilde, Denmark, National Environmental Research Institute, University of Aarhus. Technical Reports from NERI. Ref Type: Report

24. Aneja V, Schlesinger WH, Knighton R, Jennings G, Niyogi D, Gilliam W et al., editors. Regulation of Ammonia from Agriculture in Denmark - Concept of methodology. Bolger Conference Center, Potomac, Maryland, USA, 5 to 8 June 2006.: 2006.

25. Geels C, Frohn LM, Madsen PV, Hertel O. Nitrogen loads of nature areas on Bornholm and Sealand (In Danish: Kvælstofbelastning af natureområder på Bornholm og Sjælland). No xx, -57p. 2008. Roskilde, Denmark, National Environmental Research Institute, University of Aarhus. Technical Report from NERI.
Ref Type: Report

26. Frohn LM, Geels C, Madsen PV, Hertel O. Nitrogen load of nature areas in Eastern Jutland (In Danish: Kvælstofbelastning af naturområder i Østjylland). 673, -49. 2008. Roskilde, Denmark, National Environmental Research Institute, University of Aarhus. Technical Reports from NERI.
Ref Type: Report

Theobald MR, Bealey WJ, Tang YS, Sutton MA. A simple model for screening the local impacts of atmospheric ammonia. Submitted to Science of the Total Environment (2009).

van Pul WAJ, van Jaarsveld JA, Vellinga OS, van den Broek M, Smits MCJ, The VELD experiment: An evaluation of the ammonia emissions and concentrations in an agricultural area, Atmospheric Environment 2008;42(34):8086-8095.

Dragosits U, Theobald MR, Place CJ, ApSimon HM, Sutton MA The potential for spatial planning at the landscape level to mitigate the effects of atmospheric ammonia deposition. Environmental Science & Policy 9, 626-638.